Ultraprecision Machining Characteristics of Poly-crystalline Germanium

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Summary

Germanium is an excellent infrared optical material. On most occasions, single-crystalline germanium is used as optical lens substrate because its homogeneous structure is beneficial for fabricating uniform optical surfaces. In this work, we attempt to use poly crystals as lens substrates instead of single crystals, which may lead to a significant reduction in production cost. We conducted ultraprecision cutting experiments on poly-crystalline germanium to examine the microscopic machinability. The crystal orientations of specific crystal grains were characterized, and the machining characteristics of these crystal grains including surface textures, cutting forces, and grain boundary steps were investigated under various machining conditions. It was possible to produce uniformly ductile-cut surfaces across all crystal grains by using an extremely small undeformed chip thickness (≈80 nm) under high negative tool rake angles (≈−45°). This work indicates the possibility of fabricating high-quality infrared optical components from poly-crystalline germanium.

Keywords: Ultraprecision machining, Diamond turning, Ductile regime machining, Poly crystalline, Germanium, Optical surface

1. Introduction

Germanium (Ge) is an excellent infrared optical material which has high permeability and high refractive index in the infrared wavelength range. It is a major substrate material for infrared optical components with extensive applications in thermal imaging systems, dark-field optical instruments, infrared astronomical telescopes, and so on. According to its microstructure, germanium can be divided into poly crystals and single crystals. On most occasions, single-crystalline germanium (s-Ge) is used as optical substrate, because its homogeneous structure is beneficial for fabricating uniform optical surfaces. However, due to the technical difficulties in growing large-diameter s-Ge ingots, the production cost of large-diameter optical lenses is very high.

In this work, we attempt to use poly-crystalline germanium (p-Ge) as optical lens substrates to substitute s-Ge. This innovation, if succeeds, will lead to a significant reduction in costs for infrared optical components. However, germanium is a highly brittle material with strong crystallographic anisotropy. Thus, the microscopic mechanical properties vary with crystal grains, resulting in significantly different processing behaviors. This anisotropic effect will cause nonuniformity in surface quality and eventually limit the productivity of the manufacturing processes.

Among various optical manufacturing technologies, single-point diamond turning (SPDT) has been demonstrated to be capable of machining complex geometries with nanometer level accuracy. Previous studies have found that s-Ge undergoes high-pressure phase transformations which give rise to plastic deformation during indentation tests, scratching and machining (1)-(5). The feasibility for fabricating diffractive infrared lenses from s-Ge by SPDT has also been demonstrated (6). On the other hand, to date, little literature can be found on the ultra-precision machining of p-Ge. In this work, we conducted ultraprecision cutting experiments on p-Ge to examine its microscopic machinability. The crystal orientations of specific crystal grains were characterized and their machining characteristics were investigated. The critical conditions for producing uniform smooth surfaces on all crystal grains were experimentally examined.

2. Materials and Methods
2.1 Machining apparatus

Machining experiments were carried out on an ultraprecision lathe TOYODA AHP 20-25N. A schematic illustration of the lathe is shown in Fig. 1 (a). It has a hydrostatic bearing spindle and two perpendicular slide tables along the X-axis and the Z-axis. The slide table driving system has a two-level structure: a hydraulic system for coarse motion and a servomotor system for fine motion. A precision tool post is installed on the Z-axis table. This tool post can rotate in the X-Z plane and enables fine adjustment
Fig. 1 Schematic illustrations of (a) ultra-precision lathe and (b) cutting force measurement setup.

Fig. 2 Machining model.

2.2 Machining model

Straight-nosed cutting tools (7) made of single-crystal diamond were used for machining. The machining model is schematically shown in Fig. 2. The tool moves longitudinally with periodical transverse feeds, hence regular shallow grooves are generated on the workpiece surface. For this tool geometry, undeformed chip thickness \( h \) is uniform across the entire width of the cutting edge. Thus, the relationship between the surface texture and the undeformed chip thickness is unambiguous and readily studied. The relationship among undeformed chip thickness \( h \), cutting edge angle \( \kappa \) and tool feed \( f \) can be described by Eq. (1):

\[
h = f \cdot \sin \kappa
\]

Thus, by varying cutting edge angle \( \kappa \) and/or tool feed \( f \), it is possible to change the undeformed chip thickness \( h \) from the micron level to the nanometer level.

2.3 Machining conditions

A diamond tool which has a nominal rake angle of 0° and a nominal relief angle of 6° was used for cutting. The tool rake face was tilted with tapered steel blocks to obtain negative rake angles down to -45°. Due to the inclination of the tool, the relief angle was also changed, from 6° to 51°. Using negative rake...
angles was to achieve a compressive stress field ahead the cutting edge, which is essential for ductile machining of hard brittle materials \(^{(8)}\).

Three pieces of \(p\)-Ge substrates were used as workpieces. The workpieces are 10 mm in diameter, 3 mm in thickness and obtained with polished finishes. In order to characterize the distributions and orientations of crystal grains, an orientation imaging microscopy (OIM) system produced by TexSEM Laboratories, Inc. was used. Figure 3 shows a grain map and pole figures of crystal grains A, B and C, which are selected as experiment samples in this study. From the OIM results, the boundaries and the orientations of the crystal grains can be clearly identified. The workpieces were bonded to a diamond-turned aluminum blank (diameter 125 mm) using a heat-softened glue and then vacuum-chucked to the machine spindle.

Machining conditions used in the experiments are summarized in Table 1. Depth of cut \(a\) was set to 2 \(\mu\)m. Undeformed chip thickness \(h\) was varied in the range of 0 ~ 700 nm, by changing tool feed \(f\) in the range of 7 ~ 37.5 \(\mu\)m and cutting edge angle \(\kappa\) in the range of 0.15 ~ 1.45\(^{\circ}\). The rotation rate of the machine spindle was fixed to 800 rpm, consequently, the cutting speed changes in the range of 4.8 ~ 5.2 m/s. Dry cuts were performed without coolant. A Nomarski differential interference microscope, a scanning electron microscope (SEM), a laser probe scanning three-dimensional measuring machine, and an atomic force microscope (AFM) were used to examine and measure the machined surfaces. The cutting chips were also observed using the SEM.

3. Results and discussion
3.1 Surface texture

Figure 4 is a Nomarski differential interference micrograph of the machined surface near the grain boundaries of crystal grains A, B and C, as shown in Fig.3. Apparently, the surface textures of these grains are very different, some are smooth and the others are damaged by micro pits. Therefore, grain boundaries can be identified clearly among these grains. Fig.5 is the magnified micrographs of these crystal grains. The parallel bright lines seen on the surfaces are the tool marks corresponding to periodical tool feeds. In Fig 5 (a), the surface is severely damaged with numerous micro craters and cracks, the size of which ranges in the order of 1 to 10 \(\mu\)m. In Fig 5 (b), the surface is extremely smooth, without any micro-fractures. In Fig 5 (c), the surface is generally smooth, but dotted with a few micro-fractures in the order of 1 \(\mu\)m.

Germanium has a strong directional covalent bond with the diamond-cubic structure. The cleavage plane is \([111]\) and the predominant slip system is \([111][110]\). During machining \(p\)-Ge, the orientations of the cleavage planes and slip systems changes as the tool passes different crystal grains. Consequently, the cleavage/slipping behavior is location-dependent and determines whether brittle fracture or plastic deformation occurs. An analytical model of the crystallographic effect on machining behavior using the Schmid’s factor will be further discussed elsewhere in another paper.

Fig. 4 Nomarski micrograph of machined surface near grain boundaries at conditions \(\gamma = -20^{\circ}\) and \(h = 318\) nm.

Fig. 5 Magnified photographs of the crystal grains shown in Fig. 4: (a) grain A, (b) grain B and (c) grain C.
3.2 Chip morphology

Figure 6 shows the dependence of cutting force on undeformed chip thickness. These data are obtained for high-speed machining with a rake angle of –45°. The force signals showed a standard deviation around the central value. The signals were obtained using a high-speed analog recording system. As shown in Figure 6, the force signal for an undeformed chip thickness of 6.0 mm was obtained from a 1.0 mm thick workpiece. By decreasing the undeformed chip thickness, the force signal was recorded at a lower level and the force signal was obtained at a lower level. The force signal for an undeformed chip thickness of 1.0 mm was obtained from a 0.1 mm thick workpiece. By decreasing the undeformed chip thickness, the force signal was recorded at a higher level and the force signal was obtained at a higher level. The force signal for an undeformed chip thickness of 0.1 mm was obtained from a 0.01 mm thick workpiece. By decreasing the undeformed chip thickness, the force signal was recorded at a lower level and the force signal was obtained at a lower level. The force signal for an undeformed chip thickness of 0.01 mm was obtained from a 0.001 mm thick workpiece. By decreasing the undeformed chip thickness, the force signal was recorded at a higher level and the force signal was obtained at a higher level. The force signal for an undeformed chip thickness of 0.001 mm was obtained from a 0.0001 mm thick workpiece. By decreasing the undeformed chip thickness, the force signal was recorded at a lower level and the force signal was obtained at a lower level.

3.3 Micro cutting forces

Figure 7 shows the wavinesses of principal cutting force and thrust cutting force during machining at different undeformed thicknesses. The wavinesses of principal cutting force and thrust cutting force depend on crystal grains and the force signals fluctuated significantly. Those grains which have been severely damaged by brittle fractures correspond to smaller forces, and those slightly damaged correspond to larger forces. However, this crystal-grain dependence of cutting force becomes insignificant as undeformed chip thickness decreases, as shown in Figure 6. When undeformed chip thickness is further decreased to 42 nm, all crystal grains are ductile-machined, the force variation becomes very small and is not noticeable.

3.4 Grain boundary step

Surface regions near grain boundaries were measured to characterize the grain boundary steps. Figure 8 shows a Nomarski micrograph of the surface near the boundary between two adjoining crystal grains A and B, which is machined at an undeformed chip thickness of 56 nm using a –45° rake angle tool. Although both of the grains have been machined in a ductile mode, a slight dark line can be seen in the middle of the photograph, indicating the existence of a grain boundary step. Figure 8 shows an AFM image of a small region near the grain boundary. In the figure, the saw-toothed surface profile generated by periodic tool feed demonstrates a perfect transcription between the cutting edge and the workpiece.
Fig. 8 (a) Nomarski micrograph, (b) AFM image, and (c) cross-sectional profile of a grain boundary step. Machining conditions are $h=56$ nm, $\gamma=-45^\circ$. The profile in (c) is measured from P to P' indicated in (b).

Across the tool feed marks, a grain boundary step can be clearly seen, which corresponds to the dark line shown in Fig. 8 (a). Figure 8 (c) is a cross-sectional profile which is measured along the cutting direction. The grain boundary step is approximately 20 nm high.

The formation mechanism of a grain boundary step during machining is thought as schematically shown in Fig. 9. Beneath and ahead of the cutting tool, the material is subjected to severe plastic and elastic deformation, where the downward elastic deformation will recover and causes a rise in surface height after the tool pass. Because the elastic modulus depends on crystal orientations, boundary steps will then be formed after the strain releases at different degrees. Figure 10 shows the relationship between undeformed chip thickness and the heights of crystal grain boundary steps. As undeformed chip thickness increases, the boundary step height also increases. This result indicates that an extremely small undeformed chip thickness is essential for producing smooth optical surfaces without noticeable boundary steps.

### 3.5 Effects of rake angle

Tool rake angle has been known to be a key process parameter for ductile regime machining of brittle materials. Negative rake angle can produce
compressive stress field involving hydrostatic pressure which is beneficial for ductile regime material removal (8-11). In this work, tool rake angle was changed from 0 to \(-45^\circ\) to examine its effects on the machining characteristics of \(p\)-Ge.

Figure 11 shows the variations in surface roughness of crystal grains A and B machined with different rake angle tools at various undeformed chip thicknesses. The surface roughness is measured along the cutting direction and the influence of the tool feed marks is not considered; thus the surface roughness can exactly represent the orthogonal cutting behavior. From the figure, it is clearly seen that for both crystal grains, higher negative rake angle tools produce lower surface roughness, and generally the \(-45^\circ\) rake angle tool works the best. By using an extremely small undeformed chip thickness (\(\sim 80\) nm) under the \(-45^\circ\) rake angle tool, uniform ductile-cut surfaces with the nanometer level roughness were obtained for all the examined crystal grains.

4. Conclusions

In order to explore the feasibility of using poly-crystalline germanium as infrared optical lens substrates instead of single crystals, we conducted ultraprecision cutting experiments on poly-crystalline germanium to examine its microscopic machinability. The machining characteristics of various crystal grains including machined surface textures, cutting forces, and grain boundary steps were investigated under various machining conditions. Uniformly ductile-cut surfaces were obtained on all crystal grains by using an extremely small undeformed chip thickness (\(\sim 80\) nm) under high negative tool rake angles (\(-45^\circ\)). The possibility of fabricating high-quality infrared optical components from poly-crystalline germanium has been demonstrated.

Acknowledgements

This study has been partially supported by an industrial technology research grant program (04A31508) from the Japan New Energy and Industrial Technology Development Organization (NEDO).

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